Thermal conductivity of anisotropic and frustrated spin-1/2 chains

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We analyze the thermal conductivity of anisotropic and frustrated spin-1/2 chains using analytical and numerical techniques. This includes mean-field theory based on the Jordan-Wigner transformation, bosonization, and exact diagonalization of systems with $N \leq 18$ sites. We present results for the temperature dependence of the zero-frequency weight of the conductivity for several values of the anisotropy Δ. In the gapless regime, we show that the mean-field theory compares well to known results and that the low-temperature limit is correctly described by bosonization. In the antiferromagnetic and ferromagnetic gapped regime, we analyze the temperature dependence of the thermal conductivity numerically. The convergence of the finite-size data is remarkably good in the ferromagnetic case. Finally, we apply our numerical method and mean-field theory to the frustrated chain where we find a good agreement of these two approaches on finite systems. Our numerical data do not yield evidence for a diverging thermal conductivity in the thermodynamic limit in case of the antiferromagnetic gapped regime of the frustrated chain.

Introduction - Transport properties of low-dimensional spin systems have attracted recently interest both from the experimental and theoretical side. A particular motivation comes from the observation that magnetic excitations of one-dimensional spin systems significantly contribute to the thermal conductivity which is manifest in many experiments on materials such as the spin-ladder system[1,2,3] $(Sr,La,Ca)_{14}Cu_{24}O_{41}$ and the spin-chain compounds $SrCuO_2$ and Sr_2CuO_3[4]. Assuming elementary excitations to carry the thermal current and using a relaxation time ansatz for their kinetic equation one finds extremely large mean-free paths being, for example, of the order of 1000Å in $La_5Ca_9Cu_{24}O_{41}$[2]. Although the magnitude of the mean-free path is currently an issue of intense discussion, the question arises whether heat transport in low-dimensional spin systems is ballistic, i.e., whether intrinsic scattering of magnetic excitations is ineffective to render the thermal conductivity finite. From the theoretical point of view this issue is related to the value of the so-called (thermal) Drude weight[5] D_{th} which is the zero-frequency weight of the thermal conductivity κ. A nonzero value of D_{th} corresponds to a diverging thermal conductivity. This scenario is trivially realized if the energy-current operator is a conserved quantity, which is the case for the spin-1/2 Heisenberg chain[5,6]. For a number of other models like the frustrated chain, the dimerized chains or the spin ladder the energy-current operator is not conserved and the question of nonzero D_{th} is a challenging topic.

In this paper, we establish various numerical and analytical techniques to analyze the thermal Drude weight and to compute the temperature dependence of $D_{\mathrm{th}}(T)$. We study the model Hamiltonian $H = \sum_l h_l$ with the local energy-density given by

$$h_l = J\{(S_l^+ S_{l+1}^- + \mathrm{H.c.})/2 + \Delta S_l^z S_{l+1}^z + \alpha \vec{S}_l \cdot \vec{S}_{l+2}\}. \quad (1)$$

The XXZ model ($\alpha = 0$) is integrable whereas for nonzero frustration the model becomes nonintegrable. Recently, Klümper and Sakai[7] obtained $D_{\mathrm{th}}(T)$ for $\alpha = 0$ and $0 \leq \Delta \leq 1$ by using the Bethe ansatz[8] which allows us to test our approaches in this regime. Exact diagonalization of finite systems up to $N = 14$ sites has been applied by Alvarez and Gros[9] to investigate $D_{\mathrm{th}}(T)$ for the isotropic Heisenberg chain (i.e., $\Delta = 1$), the frustrated chain, and the spin ladder. Our numerical analysis goes beyond this by allowing $\Delta \neq 1$ and extension to larger systems with $N \leq 18$ sites.

Thermal conductivity - The thermal conductivity κ is defined by $\langle j \rangle = -\kappa \nabla T$ and is given by the following expression[10]:

$$\kappa(\omega) = \beta \int_0^\infty dt\, e^{-i\omega t} \int_0^\beta d\tau \langle j(-t - i\tau) j \rangle. \quad (2)$$

j is the energy-current operator[11] and $\beta = 1/T$ is the inverse temperature. The current operator satisfies the equation of continuity: $\partial_t h_l = i[H, h_l] = -(j_{l+1} - j_l)$. For exchange interaction of arbitrary range, i.e., $[h_{l\pm m}, h_l] \neq 0$ for $m \leq m_0$, this implies

$$j_l = i \sum_{m,n=0}^{m_0-1} [h_{l-m-1}, h_{l+n}]. \quad (3)$$

In our case we have $m_0 = 2$ (see Eq. (1)) leading to

$$j = \sum_l j_l = i \sum_l [h_{l-2} + h_{l-1}, h_l + h_{l+1}]. \quad (4)$$

Note that the current operator derived from Eq. (4) includes the proper limiting form for $\alpha \gg 1$ where one recovers the current operators of two decoupled chains.

The conductivity $\kappa(\omega)$ may be decomposed according to $\mathrm{Re}\,\kappa(\omega) = D_{\mathrm{th}}(T)\,\delta(\omega) + \kappa_{\mathrm{reg}}(\omega)$ into a singular part at zero frequency and a regular part $\kappa_{\mathrm{reg}}(\omega)$. The quantity of interest is the thermal Drude weight $D_{\mathrm{th}}(T)$ which

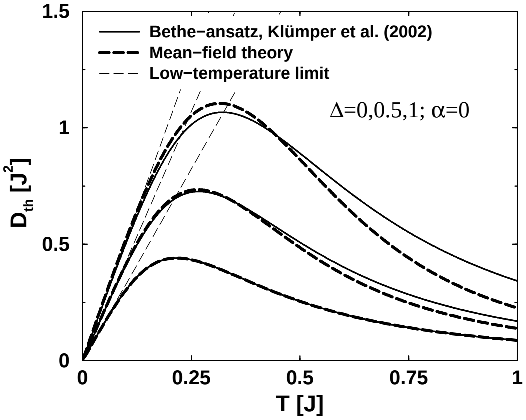

FIG. 1: $D_{\rm th}(T)$ for different values of the anisotropy $\Delta = 1, 0.5, 0$ (top to bottom) and zero frustration. Dashed lines denote results obtained by Jordan-Wigner transformation and mean-field treatment of the interaction term. Bethe-ansatz results from Ref. 7 are included in the figure (thick solid lines). Thin dashed lines show the exact result for the low-temperature limit (see Eq. (9)).

can be computed via (see, e.g., Ref. 5)

$$D_{\rm th}(T) = \frac{\pi\beta^2}{Z\,N} \sum_{\substack{m,n \\ E_m=E_n}} e^{-\beta E_m} |\langle m|j|n\rangle|^2. \qquad (5)$$

Z is the partition function and N the number of lattice sites. Note that we exclusively use periodic boundary conditions. If j is a conserved quantity, the conductivity reduces to $\kappa(\omega) = D_{\rm th}(T)\delta(\omega)$ and expression (5) simplifies to $D_{\rm th} = \pi\beta^2\langle j^2\rangle/N$.

Mean-field theory - Using a Jordan-Wigner transformation[10] the spin operators are mapped to spinless fermionic operators $c_l^{(\dagger)}$. In the case of $\Delta = 0$ and zero frustration α the corresponding Hamiltonian is diagonal in momentum space and reads $H = \sum_k \epsilon_k c_k^\dagger c_k$ with a tight-binding dispersion $\epsilon_k = -J\cos(k)$. A nonzero value of Δ or α leads to a four-fermion interaction term that can be treated approximately by Hartree-Fock (for details, see, e.g., Ref. 12), resulting in a renormalization of ϵ_k to $\tilde{\epsilon}_k = -J(1+2A(\Delta-2\alpha))\cos(k)$. The parameter $A = \frac{1}{\pi}\int_0^\pi dk\,\cos(k) f(\tilde{\epsilon}_k)$ has to be determined self-consistently where $f(\epsilon) = 1/(\exp(\beta\epsilon)+1)$ is the Fermi function. Using Eq. (5) the thermal conductivity $\kappa(\omega) = D_{\rm th}(T)\delta(\omega)$ can be computed directly. Here we focus on the case of $0 \le \Delta \le 1$ and $\alpha < \alpha_{\rm crit}$[13], which is known to exhibit gapless spinonlike excitations. Results for $D_{\rm th}(T)$ of the XXZ model are shown in Fig. 1 (thick dashed lines). For comparison Bethe-ansatz results[7] are included in the figure (solid lines). In the case of $\Delta = 0$, no approximations are necessary in the Jordan-Wigner approach and consequently, Jordan-Wigner and Bethe-ansatz results are identical. For $\Delta > 0$, the main observation is that the mean-field theory produces qualitatively the right picture of the temperature dependence of $D_{\rm th}(T)$. Both the slope of $D_{\rm th} \sim T$ at low temperatures and the position of the maximum are well predicted. Deviations at high temperatures are due to the neglect of many-particle excitations in the mean-field approximation.

Bosonization - In the continuum limit the physics of the anisotropic spin-1/2 chain at low energies is described by the Luttinger-liquid Hamiltonian[14]

$$H = \frac{1}{2}\int dx\,\left(vK(\partial_x\Theta)^2 + \frac{v}{K}(\partial_x\phi)^2\right), \qquad (6)$$

where ϕ is a bosonic field in $1+1$ dimensions and Θ is the dual field $\partial_x\Theta = \frac{1}{K}\partial_\tau\phi$. K is the Luttinger parameter and $v = (J\pi/2)\frac{\sin\gamma}{\gamma}$ is the spinon velocity where the anisotropy is parametrized via $\Delta = \cos(\gamma)$ here. The local current operator $j(x)$ is again given by the equation of continuity: $\partial_x\, j(x) = -\partial_t h(x)$. We obtain

$$j = v^2 \int dx\,\partial_x\phi(x)\partial_x\Theta(x). \qquad (7)$$

The Drude weight follows from $D_{\rm th} = \pi\beta^2\langle j^2\rangle/N$. Thus we have to evaluate the two-point function $\langle j(x,\tau)j(0,0)\rangle$, τ being the time variable. The computation is similar to the procedure for the susceptibility in Ref. 15. We change to coordinates $z = v\tau + ix$ and $\bar{z} = v\tau - ix$. By decomposing $\phi(z,\bar{z}) = \varphi(z) + \bar{\varphi}(\bar{z})$ into its chiral parts and using the respective two-point functions such as $\langle\varphi(z)\varphi(w)\rangle = -(K/4\pi)\ln(z-w)$ we obtain

$$\langle j(x,\tau)j(0,0)\rangle = -2\frac{v^2}{(4\pi)^2}\left(\frac{1}{z^4} + \frac{1}{\bar{z}^4}\right). \qquad (8)$$

Before performing the space integration the imaginary time direction is compactified by mapping the plane (z) into the strip (ζ) using $z(\zeta) = \exp(2\pi\zeta/\beta)$ leading to the replacement $v\tau \pm ix \to (v\beta/\pi)\sin(\pi\frac{v\tau\pm ix}{v\beta})$ in Eq. (8). After the change of variables $u = \tan(\pi\tau/\beta); w = -i\tan(i\pi x/(v\beta))$ we finally find

$$D_{\rm th}(T) = \frac{\pi^2}{3}\,v\,T. \qquad (9)$$

This coincides with Klümper's and Sakai's analytic expression[7] for the low-temperature limit of the XXZ model if the velocity v is equal to $v = (J\pi/2)\frac{\sin\gamma}{\gamma}$. However, the result is more generally valid for models with the continuum limit given by the Luttinger-liquid Hamiltonian.

Exact diagonalization (ED) - In this part we present our results for $D_{\rm th}(T)$ obtained by exact diagonalization for finite systems with $N \le 18$. We start with the discussion of different values of the anisotropy Δ at zero frustration. Figure 2 shows $D_{\rm th}$ for the isotropic case $\Delta = 1$, for a gapped, antiferromagnetic system ($\Delta = 10$) and in the ferromagnetic regime ($\Delta = -1, -2$). While we show in Fig. 2(a) that we reproduce the results by Alvarez and Gros[9] for system sizes of $N \le 14$, our analysis extends this case to $N \le 18$. This is due to exploiting both conservation of total S^z and momentum k in the exact

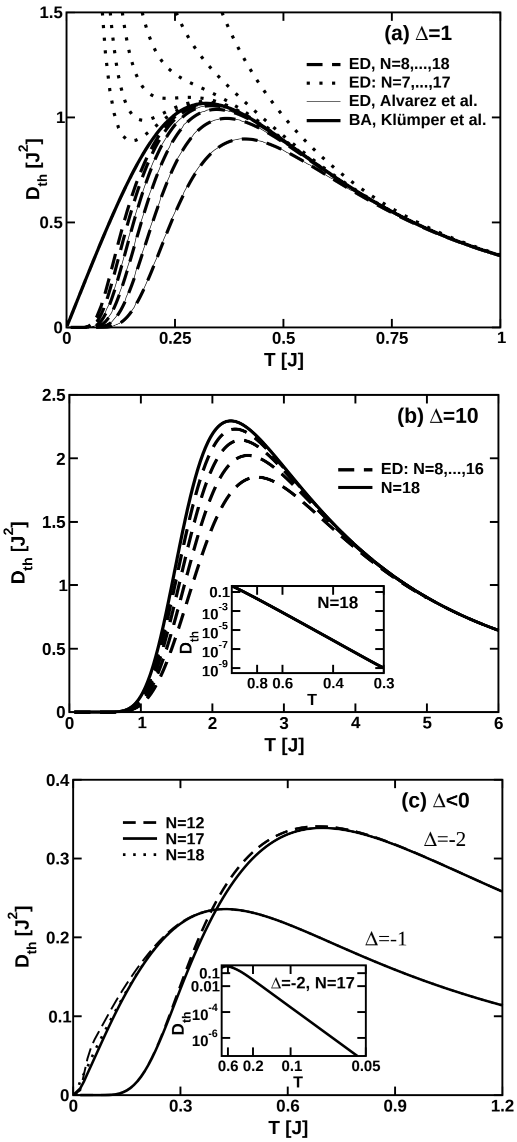

FIG. 2: Exact diagonalization (ED) for the XXZ chain: (a) Isotropic chain ($\Delta = 1$). Dashed(dotted) lines denote even(odd)-numbered systems for $N \leq 18$ sites. Bethe-ansatz results by Klümper and Sakai[7] are included in the plot (thick solid line). Thin solid lines show ED results by Alvarez and Gros[9] for $N = 8, 10, 12, 14$. (b) Antiferromagnetic, gapped regime ($\Delta = 10$). ED for $N = 8, \dots, 16$ (dashed lines), $N = 18$ (solid line). (c) Ferromagnetic regime ($\Delta = -1, -2$). Note: the thermodynamic limit is reached for $N \approx 17$. The insets of (b) and (c) display the exponential suppression of $D_{\rm th}(T)$ at low temperatures for $\Delta = 10$ and $\Delta = -2$ (in the insets, vertical axes are scaled logarithmically, horizontal axes reciprocally).

diagonalization. By comparing with the curve obtained from the Bethe ansatz[7] (solid line in Fig. 2(a)) it can be seen that for a system of $N = 18$ sites the thermodynamic limit is reached for temperatures around $T \gtrsim 0.3J$ for $\Delta = 1$. At low temperatures $D_{\rm th}(T)$ is exponentially suppressed due to the finite-size gap in the case of an even number of sites and divergent for an odd number. The latter is due to the degeneracy of the ground state in case of odd-numbered systems.

For the gapped, antiferromagnetic case we choose $\Delta = 10$, shown in Fig. 2 (b), where the finite-size effects of the two-spinon gap are small. The data for $D_{\rm th}$ are convergent for $T \gtrsim 3J$, but substantial finite-size effects are still present in the vicinity of the maximum, i.e., at small temperatures compared to the two-spinon gap $8.055126J$[16]. At low temperatures the thermal Drude weight $D_{\rm th}(T)$ is expected to be exponentially suppressed in the thermodynamic limit. In the inset of Fig. 2 (b) $D_{\rm th}(T)$ is plotted logarithmically versus $1/T$. If one fits $D_{\rm th}(T) \sim \exp(-\delta/T)$ to the numerical data at low temperatures[17] one finds $\delta = 8.056J$ for $N = 18$ sites with similar values of δ found for other N. This compares well to the two-spinon gap[16]. Hence we conclude that mainly the elementary excitations contribute to the thermal conductivity at low temperatures.

In the ferromagnetic regime ($\Delta \leq -1$) (results are shown for $\Delta = -1$ and $\Delta = -2$ in Fig. 2(c)) our main observation is that convergence with N is very good at all temperatures. For example, we find for $\Delta = -2$ that the relative difference between the finite-size data for $N = 16$ sites and $N = 17$ is negligibly small, namely $|D_{\rm th}^{N=17}(T) - D_{\rm th}^{N=16}(T)|/D_{\rm th}^{N=17}(T) < 0.008$ for $T > 0.05J$. If one extracts δ from a fit of $D_{\rm th}(T) \sim \exp(-\delta/T)$ to the numerical data[17] for $\Delta = -2$, we find $\delta \approx 0.97J$ which coincides with the one-triplet gap $-(\Delta+1)J$ that can easily be obtained from a spin-wave computation. The fast convergence is even more remarkable for the case $\Delta = -1$ where the numerical data are consistent with $D_{\rm th}(T) \sim T$ at low temperatures. In addition, there is no qualitative difference between even- and odd-numbered systems due to the ferromagnetic nature of the interaction for $\Delta \leq -1$.

Frustrated chain - Now we turn to the case of nonzero frustration. Since $[H, j] \neq 0$ here, care has to be taken about off-diagonal matrix-elements of j if degeneracies occur. However, since we use classification by momentum k and S^z degeneracies are lifted and do not play a crucial role. In Fig. 3 we show $D_{\rm th}(T)$ obtained numerically from Eqs. (4) and (5) for even system sizes with $N \leq 18$ and $\alpha = 0.35, \Delta = 1$. A central result of this paper is that, while we observe a finite Drude weight at temperatures $T > 0$ and all system sizes investigated, we still find a substantial reduction of the Drude weight with increasing system size at high T. This is in sharp contrast to the XXZ model, where finite-size effects are small at high temperatures (see e.g. Fig. 2 (a)). These observations clearly point to a vanishing of the Drude weight in the thermodynamic limit for $\alpha = 0.35$. However, the question of dissipationless thermal transport at arbitrary $\alpha > 0$ remains to be studied in more detail.

Finally, we compare our mean-field approach with numerical results on finite systems and with nonzero frustration. In Fig. 4 we present the thermal Drude weight of systems with $N = 16$ sites for $\alpha = 0, 0.05, 0.15$ and $\Delta = 1$, i.e., in the gapless regime. As is obvious from this figure, there is a good agreement between ED and the

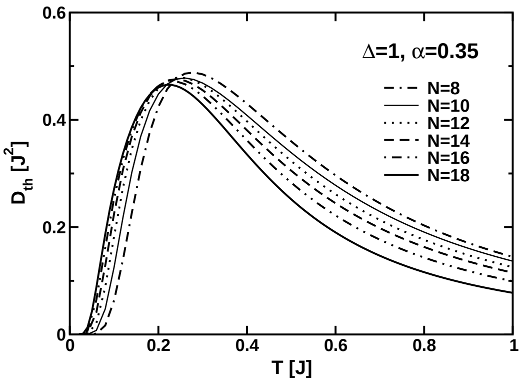

FIG. 3: Thermal Drude weight $D_{\rm th}(T)$ for the frustrated chain with $\Delta = 1, \alpha = 0.35$ for $N = 8, \ldots, 18$ sites.

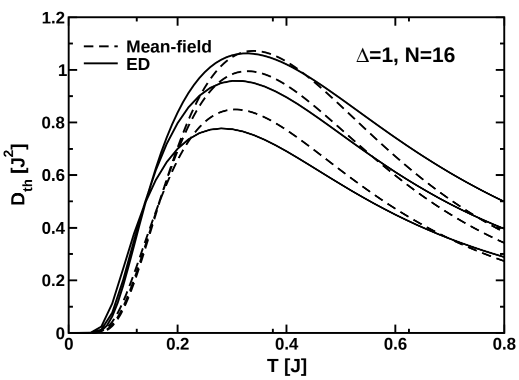

FIG. 4: Comparison between exact diagonalization (solid lines) and mean-field approximation (dashed lines) on finite systems with $N = 16$ sites for various values of $\alpha = 0, 0.05, 0.15$ (top to bottom) and $\Delta = 1$.

mean-field approach regarding the temperature dependence of the thermal Drude weight. The general features of $D_{\rm th}(T)$ are a reduction of the absolute value of $D_{\rm th}$ on increasing α, a shift of the position of the maximum to lower temperatures and thus a crossing of the curves for different α at low temperatures which are present in both the ED and mean-field results. Deviations at high temperatures are again understandable due to the neglect of many-particle excitations in the effective one-particle picture.

Conclusion - We performed a detailed analysis of the thermal Drude weight for anisotropic and frustrated spin-1/2-Heisenberg chains by using mean-field theory, bosonization and ED. In the case of the XXZ model we demonstrated the applicability of these techniques for computing the temperature dependence of the thermal Drude weight. Using ED we obtained results on finite systems of $N \leq 18$ sites for arbitrary values of the anisotropy Δ. In the ferromagnetic regime ($\Delta \leq -1$) of the XXZ chain the numerical data converge to the thermodynamic limit at arbitrary temperature for moderately small system sizes ($N \approx 18$). The analytical results compare well with the Bethe ansatz[7] in the gapless regime of the XXZ model and to our numerics in the case of the frustrated chain on finite systems. Our numerical data at $\alpha = 0.35$ mark a clear difference between the integrable XXZ case and the nonintegrable one at $\alpha = 0.35$: while in the former case the Drude weight remains finite in the thermodynamic limit we have clear indications for a vanishing Drude weight at high temperatures in the latter case. Extended analysis of these findings for frustrated and dimerized chains and spin ladders will be the subject of a forthcoming paper.

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